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MW

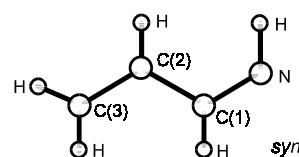
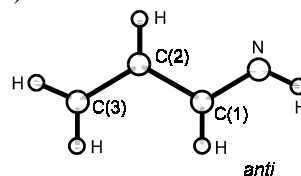
C₃H₅N

2-Propen-1-imine
3-Imino-1-propene

C_s (*syn*)
C_s (*anti*)
H₂C=CH-CH=NH

r_s	Å ^{a)}	θ_s	deg ^{a)}
C(1)–C(2)	1.454(2)	C(1)–C(2)=C(3)	122.9(2)
C(2)=C(3)	1.336(2)	C(2)–C(1)=N	121.5(5)
C(1)=N	1.274(5)	C(1)=N–H	111.7(5)
N–H	1.014(5)		

Atom	a_s [Å]	b_s [Å]
<i>anti</i>		
H(1)	2.4934	0.5184
C(1)	0.6001	0.3779
C(2)	–0.6195	–0.4130
C(3)	–1.8383	0.1338
N ^{b)}	1.7498	–0.1706
<i>syn</i>		
H(1)	1.7955	–1.0803



syn and *anti* refer to the C–C=N–H configuration. Both forms have an *s-trans* C=C–C=N conformation. The *anti* form is more stable than the *syn* form by 0.9(1) kcal mol^{–1}.

^{a)} Uncertainties were partially estimated in the original paper.

^{b)} The nitrogen coordinates are not substitution coordinates, but are determined from the assumed C–H bond length of 1.086 Å and C–C–H angle of 120° and the center-of-mass condition, see original paper.

Penn, R.E.: J. Mol. Spectrosc. **69** (1978) 373.